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[1] Z. Xie, C. Wang, K.E. deKrafft, W. Lin, *J. Am. Chem. Soc.* **2011**, *137*, 2056-2059. [2] A. Hauser, H. Riesen, R. Pellaux, S. Decurtins, *Chem. Phys. Lett.* **1996**, *261*, 313-317. [3] V.M. Russell, D.C. Craig, M.L. Scudder, I.G. Dance, *CrystEngComm* **2000**, *2*, 16-23. [4] M. Clemente-Leon, E. Coronado, C.J. Gomez-Garcia, A. Soriano-Portillo, *Inorg. Chem.* **2006**, *45*, 5653-5660. [5] S. Decurtins, H.W. Schmalte, R. Pellaux, P. Schneuwly, A. Hauser, *Inorg. Chem.* **1996**, *35*, 1451-1460. [6] R. Andres, M. Brissard, M. Gruselle, C. Train, J. Vaissermann, B. Malezieux, J.P. Jamet, M. Verdaguer, *Inorg. Chem.* **2001**, *40*, 4633-4640.

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Crystal structure of a new *N*-acyloxazolidinone

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Oxazolidinones are amongst the very few genuinely new antimicrobial classes developed in the past 30 years, being Linezolid [1] the only one marketed so far. Furthermore, their usefulness as directing groups in asymmetric synthesis has been fully tested [2]. The asymmetric alkylation reactions inspire consideration from a synthetic, mechanistic, and theoretical point of view. The development of *N*-acyloxazolidinones as chiral enolate synthons in carbon-carbon bond forming reactions has exhibited high levels of diastereoselectivity in alkylations. This compound was obtained as a result of an oxazolidinone *cross*-alkylation during Evans' asymmetric alkylation reaction.

Data from this compound were collected at 293K and at 100K in a Xcalibur Gemini diffractometer. The X-ray structure of this compound displays no noticeable modifications in crystal packing from RT to 100K. It is monoclinic and the space group is $P2_1$, with $Z = 16$.

The crystal packing shows chains along *a* crystallographic axis, formed by hydrogen bonds (-C-H...O=C-). Chains are stabilized by very weak π - π interactions between aromatic rings within the chain. According to centroid-centroid distances between two aromatic rings and the angles between the normal of the benzene ring and the centroid vector, only for one of the four pairs of centroids π - π stacking interaction may be considered. Crystal packing is formed by -H- π interactions linking chains to form layers along *b* crystallographic axis.

It was found that the chiral carbon of the 5 membered rings is R.

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[1] S.J. Brickner, D.K. Hutchinson, M.R. Barbachyn, P.R. Manninen, D.A. Ulanowicz, S.A. Garmon, K.C. Grega, S.K. Hendges, D.S. Toops, C.W. Ford, G.E. Zurenko, *J. Med. Chem.* **1996**, *39*, 673-679. [2] a) D.A. Evans, J. Bartroli, T.L. Shih, *J. Am. Chem. Soc.* **1981**, *103*, 2127-2129. b) S. Masamune, S. Choy, W. Kerdesky, F.A.J. Imperiali, *J. Am. Chem. Soc.* **1981**, *103*, 1566-1568. c) T. Hintermann, D. Seebach, *Helv. Chim. Acta.* **1998**, 2093-2126.

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Do nitrogen atoms assist the formation of racemic conglomerates?

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Racemic mixtures usually crystallize in centrosymmetric space group or in non-centrosymmetric space group having both enantiomer or their symmetry related parts in the asymmetric unit. In some cases the enantiomers form separate macroscopic crystals *i.e.* **racemic conglomerates**. This means formation of crystals with a lattice of one of the 65 space groups allowed for chiral molecules (Sohncke space groups) and $Z'=1$. Such a lattice also indicate spontaneous resolution of the racemic mixture into pure enantiomers. Formation of racemic twin crystals is also possible. Surprisingly, during our study of *tert*-amino effect [1] several compounds were found to crystallize as racemic conglomerate reproducibly, although they have been prepared by achiral route. Circular dichroism studies revealed, that while the bulk does not show Cotton effect optical rotation could be observed by choosing one single crystal in the solid state or in solution. In the case of 6,7,8,8a-tetrahydrodibenzo[e,g]pyrrolo[1,2-a]azocine-9,9(10H)-dicarbonitrile (Figure 1) not only resolution by shape chirality of the molecule occurred but resolution of a chiral carbon center was also observed. Single crystal X-ray diffraction studies of urotropine derivatives with quaternary nitrogen atom also indicated formation of racemic conglomerates. Here presence of heavy atom made it possible to determine the absolute configuration of the crystal studied. Search of the CSD (Ver. 5.32, November 2010 with updates February 2011) resulted 1054 hits for structures with Sohncke space groups and $Z'=1$. Among these hits true racemic conglomerates could be found. According to our results this phenomena is not so rare as considered generally and maybe overlooked in several cases. However, deeper understanding of formation of enantiopure or enriched crystals under achiral conditions will have far reaching consequences. The phenomena can be considered as an example for absolute asymmetric synthesis, too. Several structures with this surprising property, found in the last two years, will be presented. Each of them contained at least one tertiary or quaternary nitrogen atom. Detailed experimental studies are under way to exclude the resolution effect of traces of chiral contaminants and checking the reproducibility of crystallizations.

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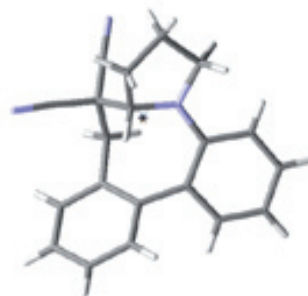


Figure 1: One of the compounds showing spontaneous resolution

[1] A. Polonka-Balint, C. Saraceno, K. Ludanyi, A. Bényei, P. Matyus, *Synlett* **2008**, 2846-2850.

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